

# A Data-Driven Approach to Computational Science

**Date:** November 17, 2016 (Thu)  
**Time:** 5:00 pm  
(light refreshments from 4:30 pm)  
**Venue:** T5, Meng Wah Complex, HKU  
**Medium:** English

by  
*Prof. Nicholas Zabaras*

*Viola D. Hank Professor of Computational Science and Engineering  
Aerospace and Mechanical Engineering  
Applied and Computational Mathematics and Statistics  
University of Notre Dame, Notre Dame, Indiana, USA*



## ABSTRACT

The future of computational science is dictated by dramatic advances in data-intensive computing, growing use of imaging, sensors and feedback control systems in guiding simulations, widespread emphasis in 'Big Data', analysis of biological systems at the cellular level, dramatic progress in rapid prototyping and nano-manufacturing, and the need to quantify uncertainties in predictions. An emerging view is that computational science will require interdisciplinary approaches towards (a) models that bridge several spatial/temporal scales (Multiscale/Multiphysics Modeling), (b) models guided by high-dimensional data (Data-Driven Simulation), and (c) models that quantify our confidence in the predictions (Uncertainty Quantification). An interdisciplinary approach to these themes poses unique challenges in particular when the focus is on engineering and scientific applications (e.g. predictive materials science, climate modeling and environmental/geological sciences, systems biology, nanoscale device design, complex interconnected systems – from the power grid to aircraft engines, and other).

We will advocate an information theoretic data-driven approach to address these challenges. In particular, we will discuss forward uncertainty propagation in high dimensions using limited data, variational approaches to stochastic coarse graining, quantifying epistemic uncertainty when using surrogate models and probabilistic graphical model and deep learning approaches for predictive modeling of multiscale and multiphysics problems. Examples will be shown from diverse areas in physical sciences and engineering.

## ABOUT THE SPEAKER

**Professor Nicholas Zabaras** joined Notre Dame's College of Engineering after serving as founding director of the Warwick Centre for Predictive Modeling at the University of Warwick and the Hans Fisher Senior Fellow with the Institute for Advanced Study at the Technical University of Munich. Prior to this, he spent 23 years serving in all academic ranks of the faculty of the Sibley School of Mechanical and Aerospace Engineering at Cornell University where he was the director of the Materials Process Design and Control Laboratory. He received his Ph.D. in Theoretical and Applied Mechanics from Cornell, after which he started his academic career at the faculty of the University of Minnesota.